

Publications

1. Stojanowski, V. et al. A Triple Mutant in the Ω -loop of TEM-1 β -lactamase Changes the Substrate Profile via a Large Conformational Change and an Altered General Base for Catalysis. *Journal of Biological Chemistry* **290**, 10382-10394 (2015).
2. Stojanowski, V. et al. Structural Basis for Different Substrate Profiles of Two Closely Related Class D β -lactamases and their Inhibition by Halogens. *Biochemistry* (2015).
3. Serbzhinskiy, D. et al. Structure of an ADP-ribosylation factor, ARF1, from Entamoeba histolytica bound to Mg²⁺-GDP. *Structural Biology and Crystallization Communications* **71**, 594-599 (2015).
4. Sarma, G.N. et al. D-AKAP2: PKA RII: PDZK1 ternary complex structure: Insights from the nucleation of a polyvalent scaffold. *Protein Science* **24**, 105-116 (2015).
5. Ogden, K.M. et al. Structural basis for 2'-5'-oligoadenylate binding and enzyme activity of a viral RNase L antagonist. *Journal of virology* (2015).
6. Marapakala, K. et al. A disulfide-bond cascade mechanism for arsenic (III) S-adenosylmethionine methyltransferase. *Biological Crystallography* **71**, 505-515 (2015).
7. Hilbert, B. et al. The Structure and Mechanism of the ATPase that Powers Viral Genome Packaging. *The FASEB Journal* **29**, LB156 (2015).
8. Edwards, T.E. et al. Crystal structures of Mycobacterial MeaB and MAA-like GTPases. *Journal of structural and functional genomics* **16**, 91-99 (2015).
9. Sippel, K.H., Vyas, N.K., Zhang, W., Sankaran, B. & Quiocho, F.A. Crystal structure of the human fatty acid synthase enoyl-acyl carrier protein-reductase domain complexed with triclosan reveals allosteric protein-protein interface inhibition. *Journal of Biological Chemistry* **289**, 33287-33295 (2014).
10. Shanker, S. et al. Structural Analysis of Determinants to HBGA Binding Specificity in GI 2 Noroviruses 3. (2014).
11. Shanker, S. et al. Structural analysis of determinants of histo-blood group antigen binding specificity in genogroup I noroviruses. *Journal of virology* **88**, 6168-6180 (2014).
12. Sastri, N.P. et al. Structural Plasticity of the Coiled-Coil Domain of Rotavirus NSP4. *Journal of virology* **88**, 13602-13612 (2014).
13. Packianathan, C. et al. Crystallization and preliminary X-ray crystallographic studies of CrArsM, an arsenic (III) S-adenosylmethionine methyltransferase from Chlamydomonas reinhardtii. *Structural Biology and Crystallization Communications* **70** (2014).
14. Nadar, S.V., Yoshinaga, M., Kandavelu, P., Sankaran, B. & Rosen, B.P. Crystallization and preliminary X-ray crystallographic studies of the ArsI C-As lyase from Thermomonospora curvata. *Acta Crystallographica Section F: Structural Biology Communications* **70**, 761-764 (2014).

15. Huang, G. Y. et al. Structural basis for cyclic-nucleotide selectivity and cGMP-selective activation of PKG I. *Structure* **22**, 116-124 (2014).
16. Huang, G. Y. et al. Neutron Diffraction Reveals Hydrogen Bonds Critical for cGMP-Selective Activation: Insights for cGMP-Dependent Protein Kinase Agonist Design. *Biochemistry* **53**, 6725-6727 (2014).
17. Carrillo, B. et al. The influenza A virus protein NS1 displays structural polymorphism. *Journal of virology* **88**, 4113-4122 (2014).
18. Bashirians, G. et al. (US Patent 8,835,183, 2014).
19. Adamski, C.J. et al. Molecular Basis for the Catalytic Specificity of the CTX-M Extended-Spectrum B-Lactamases. *Biochemistry* **54**, 447-457 (2014).
20. Zhang, Y. et al. Structural insights into the functional role of the Hcn sub-domain of the receptor-binding domain of the botulinum neurotoxin mosaic serotype C/D. *Biochimie* **95**, 1379-1385 (2013).
21. Shu, C. et al. Structural insights into the functions of TBK1 in innate antimicrobial immunity. *Structure* **21**, 1137-1148 (2013).
22. Sankaran, B., Sullivan, S.S., Haynes, D.C., Hosimer, P.C. & Yearwood, G. (US Patent 8,617,820, 2013).
23. Muhaxhiri, Z. et al. Structural basis of substrate specificity and protease inhibition in Norwalk virus. *Journal of virology* **87**, 4281-4292 (2013).
24. Huang, G. Y. et al. Structures of human PKG reveal cGMP-selectived activation mechanisms. *BMC Pharmacology and Toxicology* **14**, 1-1 (2013).
25. Driggers, C.M. et al. Cysteine dioxygenase structures from pH4 to 9: consistent cys-persulfenate formation at intermediate pH and a Cys-bound enzyme at higher pH. *Journal of molecular biology* **425**, 3121-3136 (2013).
26. Coronado, M.A. et al. Structure of the polypeptide crotamine from the Brazilian rattlesnake *Crotalus durissus terrificus*. *Acta Crystallographica Section D: Biological Crystallography* **69**, 1958-1964 (2013).
27. Brown, S.H. et al. Implementing fluorescence anisotropy screening and crystallographic analysis to define PKA isoform-selective activation by cAMP analogs. *ACS chemical biology* **8**, 2164-2172 (2013).
28. Yang, J. et al. A conserved Glu-Arg salt bridge connects coevolved motifs that define the eukaryotic protein kinase fold. *Journal of molecular biology* **415**, 666-679 (2012).
29. Jiao, G.-S. et al. Antidotes to anthrax lethal factor intoxication. Part 3: Evaluation of core structures and further modifications to the C2-side chain. *Bioorganic & medicinal chemistry letters* **22**, 2242-2246 (2012).
30. Brelidze, T.I., Carlson, A.E., Sankaran, B. & Zagotta, W.N. Structure of the C-Terminal Region of a KCNH Channel. *Biophysical Journal* **102**, 37a (2012).
31. Brelidze, T.I., Carlson, A.E., Sankaran, B. & Zagotta, W.N. Structure of the carboxy-terminal region of a KCNH channel. *Nature* **481**, 530-533 (2012).
32. Badger, J. et al. Structure determination of LpxD from the lipopolysaccharide-synthesis pathway of *Acinetobacter baumannii*. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **69**, 6-9 (2012).
33. Badger, J. et al. Structure determination of LpxA from the lipopolysaccharide-synthesis pathway of *Acinetobacter baumannii*. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **68**, 1477-1481 (2012).

34. Ajees, A.A., Marapakala, K., Packianathan, C., Sankaran, B. & Rosen, B.P. Structure of an As (III) S-adenosylmethionine methyltransferase: insights into the mechanism of arsenic biotransformation. *Biochemistry* **51**, 5476-5485 (2012).
35. Zhang, Y. et al. Structure of nitrilotriacetate monooxygenase component B from *Mycobacterium thermoresistibile*. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **67**, 1100-1105 (2011).
36. Torres, R. et al. Biochemical, structural and molecular dynamics analyses of the potential virulence factor RipA from *Yersinia pestis*. (2011).
37. Torres, R. et al. Structural insights into RipC, a putative citrate lyase subunit from a *Yersinia pestis* virulence operon. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **68**, 2-7 (2011).
38. Talley, T. T. et al. Acetylcholine binding protein-nicotinic receptor chimeras for delineating structure and determinants of ligand selectivity. *Biochemical Pharmacology* **82**, 1028-1029 (2011).
39. Sivasubramanian, V., Sankaran, B., Murali, R. & Subramanian, V. Micro algal technology to correct pH and reduce sludge in an acidic effluent from a detergent industry. *J. Algal Biomass Utln* **2**, 95-102 (2011).
40. Sippel, K.H. et al. Insights into *Mycoplasma genitalium* metabolism revealed by the structure of MG289, an extracytoplasmic thiamine binding lipoprotein. *Proteins: Structure, Function, and Bioinformatics* **79**, 528-536 (2011).
41. Shanker, S. et al. Structural analysis of histo-blood group antigen binding specificity in a norovirus GII. 4 epidemic variant: implications for epochal evolution. *Journal of virology* **85**, 8635-8645 (2011).
42. Osborne, B. W. et al. Crystal structure of cGMP-dependent protein kinase reveals novel site of interchain communication. *Structure* **19**, 1317-1327 (2011).
43. Leiby, D.J. et al. Structure of thymidylate kinase from *Ehrlichia chaffeensis*. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **67**, 1090-1094 (2011).
44. Lee, C.F. et al. X-ray crystal structure of the UCS domain-containing UNC-45 myosin chaperone from *Drosophila melanogaster*. *Structure* **19**, 397-408 (2011).
45. Jaffe, E.K. et al. Crystal Structure of *Toxoplasma gondii* Porphobilinogen Synthase INSIGHTS ON OCTAMERIC STRUCTURE AND PORPHOBILINOGEN FORMATION. *Journal of Biological Chemistry* **286**, 15298-15307 (2011).
46. Gardberg, A. et al. Structure of fructose bisphosphate aldolase from *Encephalitozoon cuniculi*. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **67**, 1055-1059 (2011).
47. Ferrell, M. et al. Structure of aldose reductase from *Giardia lamblia*. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **67**, 1113-1117 (2011).
48. Edwards, T.E. et al. Structures of a putative-class glutathione S-transferase from the pathogenic fungus *Coccidioides immitis*. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **67**, 1038-1043 (2011).
49. Brown, N.G. et al. Analysis of the binding forces driving the tight interactions between β -lactamase inhibitory protein-II (BLIP-II) and class A β -lactamases. *Journal of Biological Chemistry* **286**, 32723-32735 (2011).

50. Begley, D. W. et al. Inhibitor-bound complexes of dihydrofolate reductase-thymidylate synthase from Babesia bovis. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **67**, 1070-1077 (2011).
51. Badger, J. et al. The structure of LpxD from Pseudomonas aeruginosa at 1.3 Å resolution. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **67**, 749-752 (2011).
52. Abendroth, J. et al. BrabA. 11339. a: anomalous diffraction and ligand binding guide towards the elucidation of the function of a putative β-lactamase-like protein from Brucella melitensis. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **67**, 1106-1112 (2011).
53. Xiao, J., Worby, C.A., Mattoo, S., Sankaran, B. & Dixon, J.E. Structural basis of Fic-mediated adenylylation. *Nature structural & molecular biology* **17**, 1004-1010 (2010).
54. Talley, T. T. et al. Crystallographic comparison of nicotinic ligands in complex with the acetylcholine binding protein. *The FASEB Journal* **24**, 579-574 (2010).
55. Rinaldi, J. et al. Structure of yeast regulatory subunit: a glimpse into the evolution of PKA signaling. *Structure* **18**, 1471-1482 (2010).
56. Pornillos, O., Ganser-Pornillos, B.K., Banumathi, S., Hua, Y. & Yeager, M. Disulfide bond stabilization of the hexameric capsomer of human immunodeficiency virus. *Journal of molecular biology* **401**, 985-995 (2010).
57. McMath, L. et al. Crystallization and preliminary X-ray crystallographic analysis of a Mycobacterium tuberculosis ferritin homolog, BfrB. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **66**, 1657-1661 (2010).
58. Marapakala, K., Ajees, A.A., Qin, J., Sankaran, B. & Rosen, B.P. Crystallization and preliminary X-ray diffraction analysis of rat autotaxin. *ACTA CRYSTALLOGRAPHICA SECTION F-STRUCTURAL BIOLOGY AND CRYSTALLIZATION COMMUNICATIONS* **66**, 1050-1052 (2010).
59. Marapakala, K., Ajees, A., Qin, J., Sankaran, B. & Rosen, B.P. Crystallization and preliminary X-ray crystallographic analysis of the ArsM arsenic (III) S-adenosylmethionine methyltransferase. *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* **66**, 1050-1052 (2010).
60. Maity, K. et al. X-ray crystallographic analysis of the complexes of enoyl acyl carrier protein reductase of Plasmodium falciparum with triclosan variants to elucidate the importance of different functional groups in enzyme inhibition. *IUBMB life* **62**, 467-476 (2010).
61. Lee, C. F. et al. Crystal Structure of Drosophila Unc-45, a Putative Myosin Chaperone. *Biophysical Journal* **98**, 34a (2010).
62. Casteel, D. E. et al. A crystal structure of the cyclic GMP-dependent protein kinase IB dimerization/docking domain reveals molecular details of isoform-specific anchoring. *Journal of Biological Chemistry* **285**, 32684-32688 (2010).
63. Sankaran, B. et al. Zinc-independent folate biosynthesis: genetic, biochemical, and structural investigations reveal new metal dependence for GTP cyclohydrolase IB. *Journal of bacteriology* **191**, 6936-6949 (2009).

64. Hall, A., Sankaran, B., Poole, L. B. & Karplus, P. A. Structural changes common to catalysis in the Tpx peroxiredoxin subfamily. *Journal of molecular biology* **393**, 867-881 (2009).
65. Casteel, D.E. et al. The first crystal structure of cyclic GMP-dependent protein kinase I β dimerization/docking domain reveals molecular details of isoform-specific anchoring. *BMC Pharmacology* **9**, P6 (2009).
66. Kim, C. et al. The first crystal structure of cyclic GMP-dependent protein kinase I {beta} dimerization domain reveals the molecular features of an extended leucine/isoleucine zipper. *The FASEB Journal* **22**, 828.824 (2008).
67. Flynn, G. E., Black, K. D., Islas, L. D., Sankaran, B. & Zagotta, W. N. Structure and rearrangements in the carboxy-terminal region of SpIH channels. *Structure* **15**, 671-682 (2007).